Response to the Second Peer Review of the CMAQ Model

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This response is intended to provide clarifications and additional information to supplement the Second Peer Review of the Community Multi-scale Air Quality (CMAQ) Model, conducted for the Community Modeling Analysis Center (CMAS) at Research Triangle Park, NC during May 17-19, 2005. CMAQ is a product reflective of the on-going collaboration between the U.S. Environmental Protection Agency and the National Oceanic and Atmospheric Administration (NOAA) Atmospheric Sciences Modeling Division. The Division thanks the reviewers for their thorough, thoughtful, and constructive review and recommendations. The peer reviewers have provided valuable perspectives of the air quality modeling community needed in setting priorities and directions for the continuing development of the CMAQ modeling system. Responses are organized consonant with the structure of the Peer Review, beginning with Section 5 (Panel's Response to Charge Questions).

5. Panel's Response to Charge Questions.

<u>Charge Question 1</u>: *What is the overall quality of the applied scientific research in the CMAQ Modeling Program?*

p. 9 – *" One specific recommendation is for them to participate in meetings of the regulatory modeling community (e.g., RPO's modeling meetings) ... "*
Several CMAQ model team members have participated in the RPO's ad-hoc meteorology modeling meetings, most recently in Denver during June 2005. We do work closely with OAQPS in interacting with the RPO's and states, especially with regards to regulatory or policy-related modeling. Agency protocols require that we work through OAQPS in communications where there is significant ORD contact with regions and states on such matters.

<u>Charge Question 2</u>: *What are the strengths and weaknesses of the science being used within the components of the CMAQ development program?*

p. 10- Of the weaknesses identified, several are now the subject of active research.

a) Heterogeneous chemistry of N_2O_5
Prior to the 2002 CMAQ release, the heterogeneous pathway of nitric acid production from N_2O_5 was implicitly included in the reaction rate constant for the gas-phase reaction pathway. After conducting a literature survey in 2002 and consulting with EPA/NERL chemists on staff in NERL/HEASD, we explicitly included the heterogeneous reaction path, and set the reaction

**In partnership with the National Exposure Research Laboratory, U. S. Environmental Protection Agency* probability (parameter γ) to 0.1, as per Dentener and Crutzen (JGR, 1993), realizing there is considerable uncertainty in γ, with the model also being sensitive to its specification. In 2003, we updated the formulation for γ based upon newer work by Riemer et al. (JGR, 2003) that indicated this parameter as a function of nitrate and sulfate concentrations. We will continue to monitor the literature for new information on the heterogeneous pathway of N_2O_5, and test updates in CMAQ as warranted. We note that field experiments conducted in 2004 as part of the ICARTT study off the New England coast focused on reactions of N_2O_5 and its products during the nighttime. Hopefully, these field studies could yield new chemical information that can be included in the model.

b) Limited description of the aerosol size distribution using a modal approach with only three modes
Over the next two years, Division staff will assess the value of enhancing the representation of the aerosol size distribution in CMAQ. First, modeled size distributions obtained using the trimodal representation in CMAQ and a 9-section representation in CMAQ-UCD will each be evaluated against size- and chemically-resolved PM measurements collected during the Tampa Bay Regional Aerosol Characterization Experiment (BRACE). Second, the trimodal representation in CMAQ will be evaluated against size- and chemically-resolved PM measurements from the Pacific Northwest 2001 study via a no-cost collaboration with Environment Canada and the University of Windsor. Third, the trimodal representation in CMAQ will be evaluated against particle number distribution measurements from the Aerosol Research and Inhalation Epidemiology Study (ARIES) in Atlanta via a cooperative agreement with North Carolina State University. These evaluations will be used to identify aspects of the size representation in CMAQ that warrant improvements (e.g., size distribution of emissions, nucleation algorithms, number of modes, etc.). When determining whether or not to add more modes to the CMAQ representation, the computational cost will be weighed against the improved model performance. If resources permit in the future, a sectional version of CMAQ may be released and supported by Division staff.

c) No chemical or physical interaction between gases and the coarse mode
Work has begun on this topic. In the coming year, chemical interactions between gases and coarse sea-salt particles will be added to the model. In addition, we are monitoring scientific developments outside of EPA for later inclusion of the interactions between gases and coarse dust particles.

d) Effects of meteorology on fugitive dust emissions
The Division agrees that incorporation of a meteorologically-based fugitive dust emissions algorithm should be given a high priority. However, during the past year, we have focused our emission modeling research program on another PM emissions weakness, event-specific wildland fire emission estimates. During FY2006, we plan to renew our efforts on fugitive dust emissions by building on the work of Dr. Gillette and Dr. Shan He (now with NESCAUM). In addition, we will seek collaborative relationships with interested researchers to address this important area of uncertainty for the modeling of particulate matter.

e) Re-emissions of mercury are not treated by the model

This shortcoming is being addressed and the next official version of the CMAQ mercury model will simulate re-emission of previously deposited mercury, but only in a rather simple way. The basic scientific description of the re-emission process for mercury is still quite incomplete. We plan to base this simulated re-emission on the assumption that one-half of all atmospheric mercury deposition eventually re-emits. We are taking the simulated deposition of all forms of mercury during the year 2001 and are apportioning that flux temporally for each model grid cell based on surface temperature and solar radiation. This temporal apportionment will be based on somewhat arbitrary functions of surface temperature and solar radiation until the actual controlling factors have been described by basic scientific research.

f) Source apportionment tools (particularly for non-linear secondary PM production)
We are monitoring scientific developments outside of EPA for future inclusion of secondary source apportionment tools in the model. An ongoing effort by Georgia Tech researchers to develop a direct decoupled sensitivity method for PM (DDM-PM) is a promising candidate for inclusion in future CMAQ model releases.

g) SOA chemistry
Work within EPA has begun on developing the next generation of SOA formation mechanisms for future inclusion in the CMAQ model. SOA formation from isoprene and sesquiterpenes will be added to the model and the reversible partitioning framework of Odum and Pankow will be revised based on the results of recent smog-chamber experiments conducted at EPA and Caltech.

h) Sub-grid scale vertical transport in deep convection
In our presentation to the peer review panel, we noted that the current sub-grid scale (SGS) cloud scheme in CMAQ is simplistic and inconsistent with the treatment in the meteorology model. Therefore, this is a weakness in the model. We also included in our "To Do List": *Develop a new convective cloud model that integrates meteorological convective schemes with subgrid chemical dynamics, aqueous chemistry, wet deposition.* This is not a simple task and has not been accomplished anywhere, to our knowledge, in a mesoscale air quality model. The most straightforward approach to this problem would be to integrate the chemical and meteorological processes in an on-line air quality model such as WRF-Chem. Off-line development would follow in a consistent manner. Thus, we are collaborating with the WRF-Chem developers to help create a sophisticated integrated chemical, dynamical, and microphysical SGS cloud scheme. We have already added cloud modeling expertise to our staff and are searching for a post-doctoral researcher to conduct this research. Note that although the current SGS cloud scheme in CMAQ is simplistic and inconsistent with the meteorology model, it has been significantly improved for the 2005 release as demonstrated in the presentation to the panel.

i) Inconsistency between dry deposition module and BEIS3
We acknowledge that the inconsistencies between the vegetation and land use used in the land surface/dry deposition modeling and the biogenic emission modeling is a weakness of the current system. However, these two datasets are not as inconsistent as they first appear since BEIS land use data (BELD) are based on the same USGS land use data that are used in the LSM/Dry deposition models. BELD uses the USGS data for fine-scale (1 km) distribution of coarse phenology classifications. These data are then blended with much finer phenology, but coarser spatial scale (county level) data from other sources (USFS, USDA, etc). The reason for this is

that biogenic emissions differ by tree species far more than they do by evapotranspiration and stomatal uptake of chemical dry deposition. Thus, finer phenology classification is required for BEIS. However, the 1-km USGS database that is used by both systems is becoming increasingly out-of-date and has significant errors. We have had ongoing efforts toward replacement of this dataset with more up-to-date, higher resolution, and more accurate data, such as the National Land Cover Dataset (NLCD). Such a change will involve larger outside communities, particularly the meteorological modeling community (MM5, WRF, NCEP) since the same data must be used in the meteorological and chemical models. In the past, we have been ahead of the meteorology community and pushed them to catch up. For example, about 10 years ago we were using the 1-km USGS data and the 1-km STATSGO soil data in our MM5/LSM and dry deposition models for several years before the MM5 community added these datasets to the released MM5 system. Hopefully, we can help create a consensus agreement in the larger meteorology and air quality communities for the need for this transition.

j) Weak measurement base for the evaluation of CMAQ-Hg
We agree that the wet deposition monitoring data available in North America do not constitute a strong evaluation database for evaluating CMAQ-Hg. However, for "routine" monitoring, that is all there is for now. We are also working with EPA researchers and others outside of EPA who are collecting ambient air measurements of gaseous and particulate mercury, including RGM, in intensive field studies, in order to perform evaluations with these data.

k) Weak coupling with global chemical transport models
The linkage of CMAQ with global CTMs is a new area for us. We have worked out initial linkage between CMAQ and GEOS-Chem with collaboration from Harvard and University of Houston, and are working now on linking CMAQ with RAQMS with collaboration from NASA/Langley. These linkages must make numerous assumptions with regard to mismatches in the chemical specificity between the regional and global CTMs, and the horizontal and vertical spatial resolution in the models. Future work will explore the sensitivities of the linked modeling system results to these assumptions, as well as explore the extension of CMAQ to hemispheric applications.

p. 10 – PinG capabilities
New research and development of the PinG module is being phased out after 2005. The one exception may be in the area of including a capability for mercury in the PinG module because mercury in plumes from electric generating facilities is currently conducted at relative course spatial resolution. CMAQ's PinG module was designed for use at somewhat coarse regional scales (>20km grid size) to better represent the effects of large point source emissions on the regional scale grid. It is not designed as a near-source plume model for in-plume analysis. As grid resolutions have increased for regional applications, the need for the PinG module may be waning, except in special circumstances.

<u>Charge Question 4</u>: *What are your perceptions of the integration across different elements of the CMAQ Modeling Program (links between model development, applications, evaluation)? What is your perception of the usefulness of the CMAQ Modeling Program to the EPA, states, other customer needs and research community?*

The reviewers indicated that improvements to CMAQ which originate outside of the Division and EPA (ie. CMAQ-MADRID) should be incorporated into the core CMAQ model for best advantage to the community, rather than reinserted into each new CMAQ release. The process of adding, testing, and thoroughly evaluating new developments in CMAQ is extensive and time-consuming, modulated by available resources. Consequently, CMAS devised a multi-version repository where research versions of CMAQ are available to users while the process of improving the core release continues.

The reviewers suggested that CMAQ developers and evaluators interact more directly with RPO, state, and local model users, including by attendance at RPO modeling conferences and identifying client states, in order to obtain more user feedback. Because of the established organizational roles and structure within EPA, this contact will need to be accomplished in conjunction with the EPA Office of Air Quality Planning and Standards. Hence, we will request OAQPS to include members of the Division's CMAQ team in meetings with regional modelers and RPOs.

Charge Question 5: *Are there modeling research areas that are not being addressed or are given insufficient attention with the CMAQ Modeling Program? Are there current areas of research emphasis that might be given lower priority or eliminated? For the resources available to the CMAQ Modeling Program, are they being used in an effective manner in terms of the choice and quality of research being conducted?*

The reviewers suggested that more attention might be given to evaluating model performance by comparing model predictions with observed concentrations due to changes in emissions – for example weekday/weekend differences. This kind of "dynamic evaluation" is being developed by the Division. However, because of the large number of parameters and the strong, often overpowering, effect of meteorology, several years of model outputs are necessary to complete a meaningful evaluation.

The reviewers suggest that addition of another chemical mechanism be approached cautiously and in response to the needs of the community. Accordingly, work is underway on updating the CB4 chemical mechanism to CB4+ or CB5, in response to current knowledge and the need to accommodate more chemical species in air quality modeling, particularly for air toxins.

p. 15 – "… the fine-scale dynamics, including plume rise from vehicle exhausts may need to be considered."
Simulating the temporal and spatial variability of mobile emissions continues to challenge the application of CMAQ in urban areas. The Division agrees that plume rise from vehicle exhaust may extend above layer 1 of the model in certain circumstances, such as when high-resolution modeling for urban toxics is performed. Model sensitivity and evaluation studies of CMAQ at grid sizes approaching 1 km are planned for applications centered over Houston. If resources allow, we will examine the sensitivity of CMAQ to vehicular exhaust plume rise and assess whether changes are warranted in the current modeling approach.

Using a no-cost collaboration with Duke University and the State of Delaware, the Division is examining high-resolution pollutant concentrations collected from a mobile van driven in

Wilmington, Delaware during spring 2005. An analysis of these data, which is planned for early FY2006, should offer some insight on the temporal and spatial variability of concentrations in an urban area. In addition, Dr. Vlad Isakov (AMD) has been asked by the California Air Resources Board and the California Energy Commission to help design a Saturation Monitoring Study near Los Angeles. This study would include the deployment of several dozen monitors across a neighborhood-scale area, and the data from these monitors would assist evaluation and development of fine-scale modeling tools in the CMAQ system.

"… incorporate the most up-to-date cloud parameterization scheme in CMAQ…"
We have collaborated for many years with the University of Alabama at Huntsville on assimilation of satellite data for surface solar radiation, photolysis, and convective cloud effects into the meteorological and chemical modeling systems. The value of these techniques has been clearly established. Only resource limitations have prevented implementation in our operational systems. We continue to search for ways to accomplish this work through collaboration on research proposals with UAH.

The need for more sophisticated SGS cloud treatment and our efforts in this area are discussed above. The use of SGS schemes at finer resolutions (1-5 km) has been a hot topic of late. We have often noted problematic wind fields when modeling without SGS schemes at high resolution. Now that the meteorological modeling community is interested in this issue, primarily because of effects on convective precipitation, we hope that progress will made in this area.

p. 16 – "No four-dimensional data assimilation has been initiated (for WRF) … "
An initial effort to implement four dimensional data assimilation (nudging) into the WRF model has, in fact, begun. EPA/AMD has supported both Penn State and NCAR in this effort. AMD also has one staff member working on WRF nudging. Early results have been presented by Dr. David Stauffer (Penn State) at the most recent WRF Model Workshop in June 2005. (also, see p. 5 - 3rd bullet)

6. **PM Model Development and Evaluation – Detailed Questions and Panel's Response**

p. 18 - Visibility calculations - Current versions of CMAQ already have built-in visibility estimates (in deciviews), output as hourly 2-D fields, based on the aerosol predictions. Visibility is calculated by two distinct methods: (1) using the Mie theory and the estimated size distributions of the aerosols and (2) by the IMPROVE approximation methods based on mass of speciated components.

8. **Air Toxics Modeling – Detailed Questions and Panel's Response**

One of the objectives of the air toxics modeling version of CMAQ is to follow the same community distribution model as we have for past criteria pollutant versions of CMAQ. We have been working with state and regional EPA offices to implement the model prior to its public release. Application of CMAQ to toxic air pollutants is a new area for us and we would welcome an opportunity to participate in field studies such as MATES-III, which would also afford us user feedback on real-world applications and access to data that we can use to evaluate the model predictions. Our only hesitation is the limited size of our modeling team and our budget – participation in a field study would have to weighed against other priorities of EPA, such as the National Air Toxics Assessment (NATA), local-scale assessments for EPA's accountability standards, or multi-pollutant control studies. We thank the reviewers for mentioning MATES-III and we will keep it as a high priority area if resources allow.

We are counting on an updated 2002 Canadian toxics inventory for creating emissions in CMAQ simulations of the 2002 NATA. This inventory will be particularly critical because the 2002 assessment will include greater resolved analysis of several urban areas, including Detroit, so we won't be able ignore cross-border transport of pollutants. The air toxics modeling team will keep aware of developments in this inventory.

p. 25. – Question 1, Inhalation pollutants - We thank the reviewers for their suggestions on alternative pollutants for modeling. Diesel PM is a compound that we have been considering including because it has been identified by other EPA studies as a regional driver for non-cancer effects, and we could build on existing aerosol work in CMAQ. Based on the reviewer's comments and requests from state and regional EPA offices, we are looking into including chromium in the next version of the model – if we have enough confidence in the emission inventories and the aqueous chemistry. The reviewer's suggestion for modeling pesticides is of interest to the team. Although the Agency has not been able to support such efforts lately, beyond earlier work with atrazine, CMAQ with toxics is a tool that can be put to the use of modeling pesticides when the issue does come to the forefront.

p. 25 – Question 2, Evaluation of toxic pollutant modeling results. We appreciate the suggestions of using surrogates as well as better characterizing the monitoring sites. We have not yet explored the use of surrogates but this might give us a larger set of data for comparison, if we could get proper surrogates identified. Given the lack of monitoring data, and the high variability in the data, we also might try in future evaluations to focus our efforts on fewer sites, but on identifying more representative sites as opposed to throwing all the data and predictions into the same analysis.